

WEST Search History

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DATE: Wednesday, July 21, 2004

Hide?	<u>Set</u> <u>Name</u>	<u>Query</u>	<u>Hit</u> <u>Count</u>
	<i>DB=PGPB,USPT; PLUR=YES; OP=ADJ</i>		
<input type="checkbox"/>	L13	l12 and organic acid	57
<input type="checkbox"/>	L12	l11 and (tetrahydrofuran or THF or dimethylformamide or DMF or \$nitrile or toluene or benzene)	57
<input type="checkbox"/>	L11	l10 and \$solvent	57
<input type="checkbox"/>	L10	l8 and l9	57
<input type="checkbox"/>	L9	\$butoxide or \$amylate	25775
<input type="checkbox"/>	L8	l7 and (base or basic\$)	60
<input type="checkbox"/>	L7	l5 and (hydrogen chloride or HCl or hydrochloric acid)	60
<input type="checkbox"/>	L6	ketosulfoxonium\$	0
<input type="checkbox"/>	L5	l3 and l4	60
<input type="checkbox"/>	L4	\$sulfoxonium\$	1488
<input type="checkbox"/>	L3	l1 and l2	425
<input type="checkbox"/>	L2	carboxylic acid\$ or ester	432620
<input type="checkbox"/>	L1	\$chloroketone	472

END OF SEARCH HISTORY

d his

(FILE 'HOME' ENTERED AT 20:53:25 ON 21 JUL 2004)

FILE 'REGISTRY' ENTERED AT 20:53:49 ON 21 JUL 2004

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 9 S L1 FULL

FILE 'CASREACT' ENTERED AT 20:54:43 ON 21 JUL 2004

L4 STRUCTURE UPLOADED

L5 0 S L4

L6 0 S L4 FULL

FILE 'CAPLUS' ENTERED AT 20:55:18 ON 21 JUL 2004

L7 2 S L3

L8 591 S ?HALOKETONE OR ?CHLOROKETONE?

L9 76 S L8 AND ?ESTER

L10 930 S ?SULFOXONIUM?

L11 2 S L9 AND L10

L12 3 S L8 AND L10

L13 17 S L9 AND (HYDROCHLORIC ACID OR HYDROGEN CHLORIDE OR HCL)

L14 16 S L13 AND (CARBOXYLIC ACID? OR ESTER)

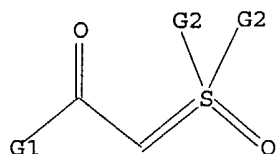
L15 1 S L14 AND ?SULFOXONIUM?

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



G1 Cb,Hy,Ak

G2 Cb,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 20:54:03 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 5120 TO ITERATE

19.5% PROCESSED 1000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 98110 TO 106690

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 20:54:07 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 103266 TO ITERATE

100.0% PROCESSED 103266 ITERATIONS
SEARCH TIME: 00.00.02

9 ANSWERS

L3 9 SEA SSS FUL L1

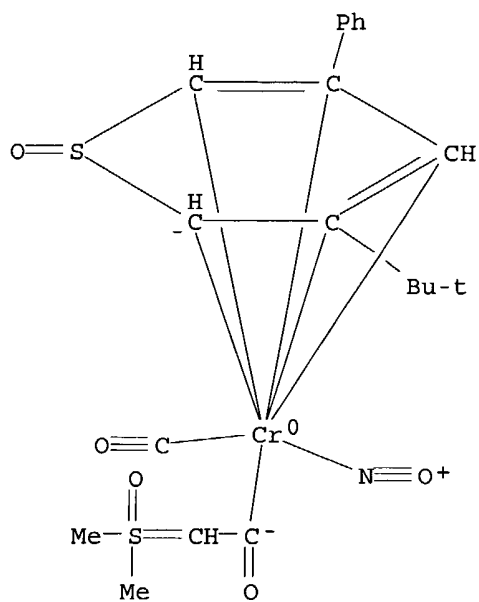
=> d scan

L3 9 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

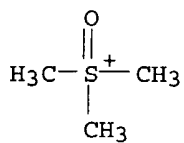
IN Sulfoxonium, trimethyl-, carbonyl[(2,3,4,5,6-η)-3-(1,1-dimethylethyl)-1-oxido-5-phenyl-2H-thiopyran-2-yl](dimethyloxosulfur)nitrosyl[μ-(1-oxo-1-ethanyl-2-ylidene)]chromate(1-) (9CI)

MF C20 H24 Cr N O5 S2 . C3 H9 O S

CM 1

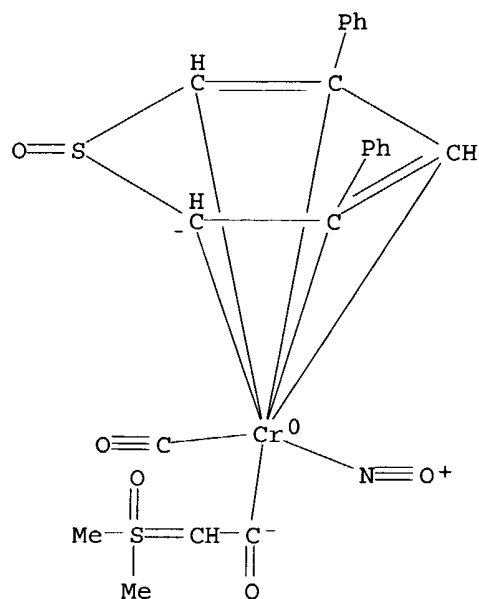


CM 2

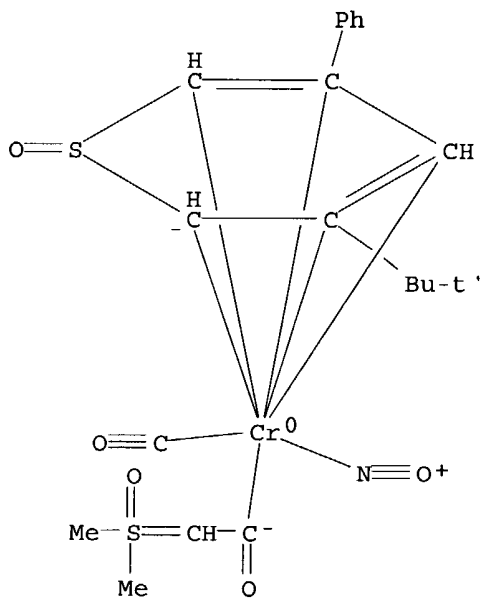


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

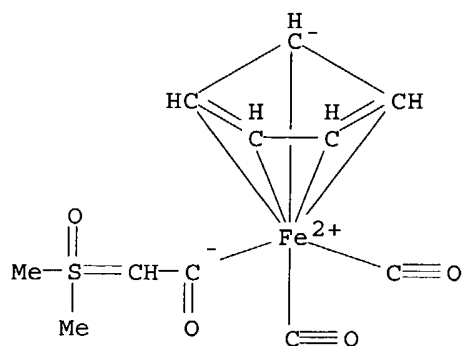
L3 9 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Chromate(1-), carbonyl(dimethyloxosulfur)[(2,3,4,5,6-η)-1-oxido-3,5-diphenyl-2H-thiopyran-2-yl]nitrosyl[μ-(1-oxo-1-ethanyl-2-ylidene)]-(9CI)
 MF C22 H20 Cr N O5 S2
 CI CCS, COM



L3 9 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Chromate(1-), carbonyl[(2,3,4,5,6-η)-3-(1,1-dimethylethyl)-1-oxido-5-phenyl-2H-thiopyran-2-yl] (dimethyloxosulfur)nitrosyl[μ-(1-oxo-1-ethanyl-2-ylidene)]- (9CI)
 MF C20 H24 Cr N O5 S2
 CI CCS, COM



L3 9 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Iron, dicarbonyl(η5-2,4-cyclopentadien-1-yl) (dimethyloxosulfur) [μ-(1-oxo-1-ethanyl-2-ylidene)]- (9CI)
 MF C11 H12 Fe O4 S
 CI CCS



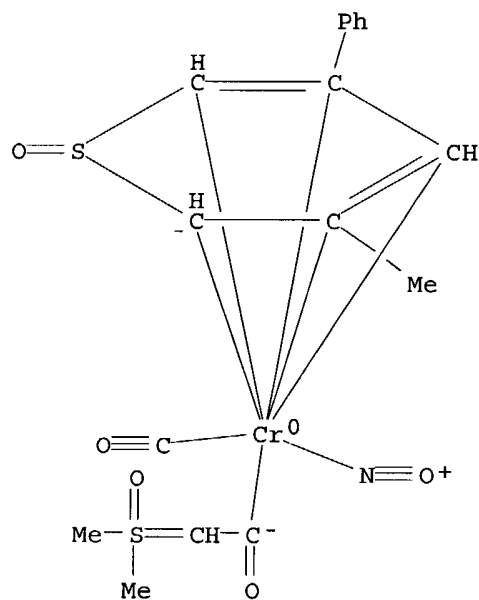
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L3 9 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

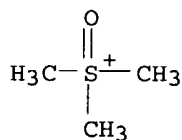
IN Sulfoxonium, trimethyl-, carbonyl(dimethyloxosulfur)[(2,3,4,5,6-η)-3-methyl-1-oxido-5-phenyl-2H-thiopyran-2-yl]nitrosyl[μ-(1-oxo-1-ethanyl-2-ylidene)]chromate(1-) (9CI)

MF C17 H18 Cr N O5 S2 . C3 H9 O S

CM 1



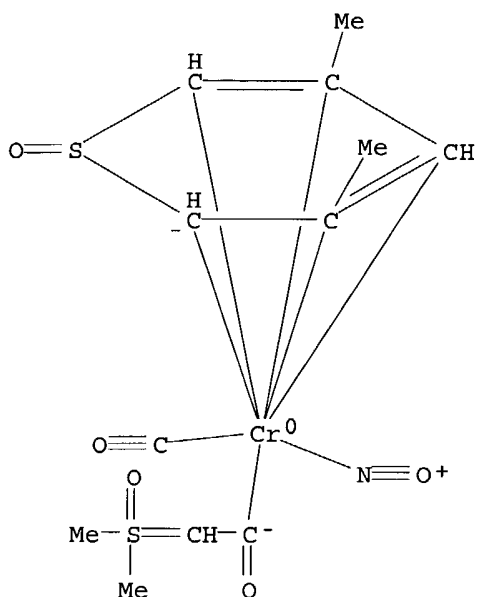
CM 2



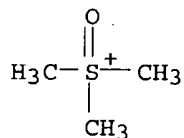
L3 9 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN Sulfoxonium, trimethyl-, carbonyl(dimethyloxosulfate)[(2,3,4,5,6-η)-3,5-dimethyl-1-oxido-2H-thiopyran-2-yl]nitrosyl[μ-(1-oxo-1-ethenyl-2-

ylidene)]chromate(1-) (9CI)
 MF C12 H16 Cr N O5 S2 . C3 H9 O S
 CM 1



CM 2



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file casreact
 COST IN U.S. DOLLARS
 FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
155.84	156.05

FILE 'CASREACT' ENTERED AT 20:54:43 ON 21 JUL 2004
 USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
 COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications.

FILE CONTENT:1840 - 18 Jul 2004 VOL 141 ISS 3

 *
 * CASREACT now has more than 8 million reactions *
 *

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>

Uploading C:\Program Files\Stnexp\Queries\771.str

L4 STRUCTURE UPLOADED

=> d

L4 HAS NO ANSWERS

L4 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s l4

SAMPLE SEARCH INITIATED 20:55:06 FILE 'CASREACT'

SCREENING COMPLETE - 0 REACTIONS TO VERIFY FROM 0 DOCUMENTS

100.0% DONE 0 VERIFIED 0 HIT RXNS 0 DOCS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED VERIFICATIONS: 0 TO 0

PROJECTED ANSWERS: 0 TO 0

L5 0 SEA SSS SAM L4 (0 REACTIONS)

=> s l4 full

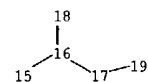
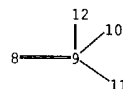
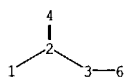
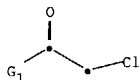
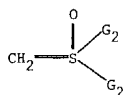
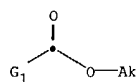
FULL SEARCH INITIATED 20:55:10 FILE 'CASREACT'

SCREENING COMPLETE - 727 REACTIONS TO VERIFY FROM 44 DOCUMENTS

100.0% DONE 727 VERIFIED 0 HIT RXNS 0 DOCS

SEARCH TIME: 00.00.01

L6 0 SEA SSS FUL L4 (0 REACTIONS)



chain nodes :

1 2 3 4 6 8 9 10 11 12 15 16 17 18 19

chain bonds :

1-2 2-3 2-4 3-6 8-9 9-10 9-11 9-12 15-16 16-17 16-18 17-19

exact/norm bonds :

1-2 2-3 2-4 3-6 9-10 9-11 9-12 15-16 16-18

exact bonds :

8-9 16-17 17-19

G1:Cb,Hy,Ak

G2:Cb,Ak

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 6:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS

12:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS

fragments assigned product role:

containing 15

fragments assigned reactant/reagent role:

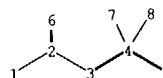
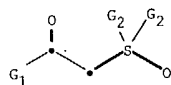
containing 1

containing 8

Element Count :

Node 6: Limited

C,C1-5



chain nodes :

1 2 3 4 5 6 7 8

chain bonds :

1-2 2-3 2-6 3-4 4-5 4-7 4-8

exact/norm bonds :

1-2 2-6 3-4 4-5 4-7 4-8

exact bonds :

2-3

G1:Cb,Hy,Ak

G2:Cb,Ak

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS